The Application of the SEDCAM Sediment Attenuation Model to Nonpolar Organic Compounds

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Abstract
The SEDCAM sediment attenuation model incorporates three processes occurring in the mixed sediment layer: accumulation, burial, and loss from diffusion or degradation. It has been used in program guidance for the Washington Sediment Management Standards to evaluate natural recovery at hazardous waste sites and has been applied to Puget Sound sediments for evaluating potential for recontamination after source control implementation. The model has been typically applied to sediments in Puget Sound using bulk (dry-weight normalized) sediment concentrations of substances. The model can be used for nonionic, nonpolar organic compounds by adjusting for carbon-normalized concentrations. The adjustment consists of multiplying the term expressing the rate of mass accumulation (M) by the concentration of total organic carbon concentration in the depositing particles and multiplying the term expressing the total accumulation of mixed sediment (S) by the total organic carbon concentration in the mixed sediment layer.

Introduction

The SEDCAM Model
Jacobs, Barrick, and Ginn (1988) developed the SEDCAM sediment attenuation model to incorporate three processes important in projecting future sediment concentrations:

- burial
- mixing
- loss by diffusion and/or degradation

Figure 1 shows a schematic diagram of the model.

The following equation defines the SEDCAM model:

$$C = \frac{M}{(M + kS)} \cdot C_i \cdot \left[1 - e^{\frac{-(kS+M)t}{S}} \right] + C_0 \cdot e^{\frac{-(kS+M)t}{S}}$$

where

C	=	concentration of substance of interest (µg/kg)
C_i	=	concentration of substance of interest in freshly deposited sediment (µg/kg)
C_0	=	concentration of substance of interest in mixed layer at t = 0 (µg/kg)
M	=	rate of mass accumulation of solid material in sediments (g/cm^2-yr)
S	=	total accumulation of sediments in the surface mixed layer (g/cm^2)
k	=	combined first-order rate constant for loss by diffusion and degradation (yr^{-1})
t	=	time in years

In its program guidance, the Washington Department of Ecology has adopted this model to evaluate natural recovery of sediments at hazardous waste sites (Ecology 1991). Schock and Shuman (undated) have applied the model, with some refinements, to evaluate potential for recontamination after sediment cleanup at the Diagonal combined sewer overflow (CSO) discharging into the Duwamish River.

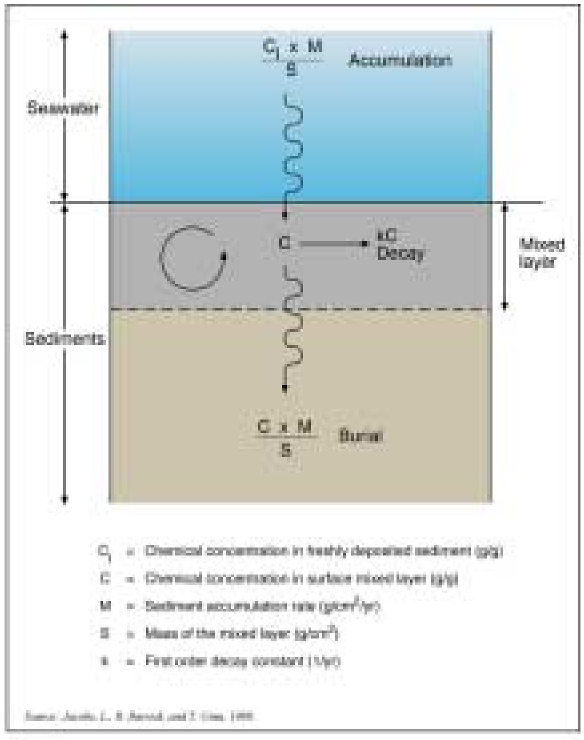

Figure 1 Schematic processes controlling chemical concentrations in surface sediments.

Rationale for Carbon-Normalized Concentrations
The U.S. Environmental Protection Agency (1989) and the State of Washington (Michelsen 1992) recommend using carbon-normalized sediment concentrations when evaluating the environmental effects of nonpolar, nonionic organic compounds. Carbon-normalized concentrations are typically expressed as "mg/kg-organic carbon" and are produced by dividing the bulk sediment concentration of a compound by the organic carbon concentration in the sediments. Owing to the specific chemical interactions between these types of organic compounds and the organic carbon in sediment, carbon-normalized concentrations better express the toxicity and other environmental effects of nonpolar organic compounds. As a result, many sediment quality criteria are expressed in carbon-normalized concentrations. The use of carbon-normalized concentrations adds an element to the application of the SEDCAM model beyond the broader bulk or dry-weight normalized concentrations used for inorganic substances or polar organic compounds.

Rationale for Adjustment to SEDCAM
However, for cases where the carbon-normalized concentrations of the substance of interest and the organic carbon concentration of the freshly depositing sediment and the sediment in the mixed layer all vary, the model requires adjustment. Such a circumstance may occur when non-native sediment is being evaluated (e.g., dredge spoils) or when a change in the organic loading is anticipated (e.g., a new discharge of wastewater containing elevated levels of organic carbon).

Objective
The objective of this poster is to derive an adjustment to the SEDCAM model to incorporate carbon-normalized concentrations for nonpolar organic compounds, allowing concentrations of organic carbon and bulk chemical concentration to vary independently.

Methods

The following equation describes the SEDCAM model:

$$\frac{dC}{dt} = \frac{C_i \cdot M}{S} - \frac{C \cdot M}{S} - kC$$

change in concentration over time = accumulation – burial - loss

where

C	=	concentration of substance of interest (μg/kg)
C_i	=	concentration of substance of interest in freshly deposited sediment (μg/kg)
M	=	rate of mass accumulation of solid material in sediments (g/cm^2-yr)
S	=	total accumulation of sediments in the surface mixed layer (g/cm^2)
k	=	combined first-order rate constant for loss by diffusion and degradation (yr^{-1})
t	=	time in years

Because the rate of mass of accumulation (M) determines the input of organic carbon to the mixed layer in the SEDCAM model, that term is multiplied by the organic carbon concentration of the freshly depositing sediments. Because the total accumulation of sediments in the mixed layer (S) determines the organic carbon content of the mixed layer in the SEDCAM model, that term is multiplied by the organic carbon concentration of the mixed layer. The “g”-units in M and S are the dry-weight normalized (bulk) mass units of the input material and the mixed layer, respectively. The organic carbon concentrations are expressed as “g-organic carbon/g-dry-weight normalized sediment” and the denominator of this unit cancels the respective “g”-units in M and S. [Derivation available on request.]

Results

The resulting equation for SEDCAM incorporating the adjustment for carbon-normalized concentrations is:

$$C' = \frac{M \cdot \mathbf{oc}_{dep}}{(M \cdot \mathbf{oc}_{dep} + kS \cdot \mathbf{oc}_{mix})} \cdot C'_i \cdot \left[1 - e^{\frac{-(kS \cdot \mathbf{oc}_{mix} + M \cdot \mathbf{oc}_{dep})t}{S \cdot \mathbf{oc}_{mix}}}\right] + C'_0 \cdot e^{\frac{-(kS \cdot \mathbf{oc}_{mix} + M \cdot \mathbf{oc}_{dep})t}{S \cdot \mathbf{oc}_{mix}}}$$

where

C'	=	carbon-normalized concentration of compound of interest (μg/kg organic carbon)
C'_i	=	carbon-normalized concentration of compound of interest in freshly deposited sediment (μg/kg organic carbon)
C'_0	=	carbon-normalized concentration of compound of interest in mixed layer at t = 0 (μg/kg organic carbon)
$\mathbf{oc}_{dep}$	=	organic carbon concentration of freshly deposited sediment (percent)
$\mathbf{oc}_{mix}$	=	organic carbon concentration of sediment in mixed layer (percent)
M	=	rate of mass accumulation of solid material in sediments (g/cm^2-yr)
S	=	total accumulation of sediments in the surface mixed layer (g/cm^2)
k	=	combined first-order rate constant for loss by diffusion and degradation (yr^{-1})
t	=	time in years

Conclusions and Further Work

Adjusting the parameters of the SEDCAM model allows application to organic compounds whose environmental effects are best expressed by carbon-normalized concentrations in cases of varying concentrations of the organic compound of interest and of the organic carbon concentration in freshly depositing sediment and in the mixed layer. The adjustments comprise measuring total organic carbon (TOC) in the existing mixed sediment layer and in the depositing sediment layer in addition to the organic compound of interest. Modern, comprehensive sediment investigations typically include these analyses when studying nonpolar organic compounds.

This adjustment corresponds to expressing the SEDCAM model in a carbon-based system.

Organic carbon typically decays in sediments, altering the carbon-normalized concentration. This adjustment has made no provision for such decay and treats the organic carbon as conservative. It would be helpful to incorporate a provision for the decay of organic carbon.

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References

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Appendix: Derivation of Adjustment for Carbon-Normalized Concentrations

The original formulation of the SEDCAM model as a differential equation is

(1) $$\frac{dC}{dt} = \frac{C_i \cdot M}{S} - \frac{C \cdot M}{S} - kC$$

change in concentration over time = accumulation – burial - loss

where

C	=	concentration of substance of interest (µg/kg)
C_i	=	concentration of substance of interest in freshly deposited sediment (µg/kg)
M	=	rate of mass accumulation of solid material in sediments (g/cm^2-yr)
S	=	total accumulation of sediments in the surface mixed layer (g/cm^2)
k	=	combined first-order rate constant for loss by diffusion and degradation (yr^{-1})
t	=	time in years

A dimensional analysis can be performed by inserting the respective units:

(2) $$\frac{dC}{dt} = \frac{C_i \dfrac{\mu g(C)}{kg(dws)_{dep}} \cdot M \dfrac{g(dws)_{dep}}{cm^2 \cdot y}}{S \dfrac{g(dws)_{mix}}{cm^2}} - \frac{C \dfrac{\mu g(C)}{kg(dws)_{mix}} \cdot M \dfrac{g(dws)_{mix}}{cm^2 \cdot y}}{S \dfrac{g(dws)_{mix}}{cm^2}} - k \cdot C \frac{\mu g(C)}{kg(dws)_{mix}}$$

where

$\mu g(C)$	=	micrograms of substance C, the organic compound of interest
$kg(dws)_{dep}$	=	kilograms of freshly depositing dry-weight normalized (bulk) sediment
$g(dws)_{dep}$	=	grams of freshly depositing dry-weight normalized (bulk) sediment
$kg(dws)_{mix}$	=	kilograms of mixed-layer dry-weight normalized (bulk) sediment
$g(dws)_{mix}$	=	grams of mixed-layer dry-weight normalized (bulk) sediment

The following equation describes the proposed adjustment for incorporating organic carbon and carbon-normalized concentrations:

(3) $$\frac{dC'}{dt} = \frac{C_i' \cdot M \cdot \mathbf{oc}_{dep}}{S \cdot \mathbf{oc}_{mix}} - \frac{C' \cdot M \cdot \mathbf{oc}_{dep}}{S \cdot \mathbf{oc}_{mix}} - kC'$$

where

C'	=	carbon-normalized concentration of compound of interest (µg/kg organic carbon)
C'_i	=	carbon-normalized concentration of compound of interest in freshly deposited sediment (µg/kg organic carbon)
$\mathbf{oc}_{dep}$	=	organic carbon concentration of freshly deposited sediment (g/g or decimal fraction)
$\mathbf{oc}_{mix}$	=	organic carbon concentration of sediment in mixed layer (g/g or decimal fraction)

Multiplying each of the *(dws)* terms by its respective organic carbon concentration yields:

(4)

$$\frac{dC'}{dt}=\frac{C_i'\dfrac{\mu g(C)}{kg(dws)_{dep}\dfrac{g(OC)_{dep}}{g(dws)_{dep}}}\cdot M\dfrac{g(dws)_{dep}\dfrac{g(OC)_{dep}}{g(dws)_{dep}}}{cm^2\cdot y}}{S\dfrac{g(dws)_{mix}\dfrac{g(OC)_{mix}}{g(dws)_{mix}}}{cm^2}}-\frac{C'\dfrac{\mu g(C)}{kg(dws)_{mix}\dfrac{g(OC)_{mix}}{g(dws)_{mix}}}\cdot M\dfrac{g(dws)_{mix}\dfrac{g(OC)_{mix}}{g(dws)_{mix}}}{cm^2\cdot y}}{S\dfrac{g(dws)_{mix}\dfrac{g(OC)_{mix}}{g(dws)_{mix}}}{cm^2}}-k\cdot C'\frac{\mu g(C)}{kg(dws)_{mix}\dfrac{g(OC)_{mix}}{g(dws)_{mix}}}$$

where

$g(OC)_{dep}$	=	grams of freshly depositing organic carbon
$g(OC)_{mix}$	=	grams of mixed-layer organic carbon

Canceling terms simplifies the equation to

(5)

$$\frac{dC'}{dt}=\frac{C_i'\dfrac{\mu g(C)}{kg(OC)_{dep}}\cdot M\dfrac{g(OC)_{dep}}{cm^2\cdot y}}{S\dfrac{g(OC)_{mix}}{cm^2}}-\frac{C'\dfrac{\mu g(C)}{kg(OC)_{mix}}\cdot M\dfrac{g(OC)_{mix}}{cm^2\cdot y}}{S\dfrac{g(OC)_{mix}}{cm^2}}-k\cdot C'\frac{\mu g(C)}{kg(OC)_{mix}}$$

which is model expressed in a carbon based system

The proposed solution to this differential equation is the adjustment of the original SEDCAM model:

(6)

$$C'=\frac{M\cdot\mathbf{oc}_{dep}}{(M\cdot\mathbf{oc}_{dep}+kS\cdot\mathbf{oc}_{mix})}\cdot C_i'\cdot\left[1-e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}\right]+C_0'\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}$$

To demonstrate that this proposed adjustment solves the model differential equation, take the first time derivative:

(7)

$$\frac{dC'}{dt}=\frac{(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})}{S\cdot\mathbf{oc}_{mix}}\cdot\frac{M\cdot\mathbf{oc}_{dep}}{(M\cdot\mathbf{oc}_{dep}+kS\cdot\mathbf{oc}_{mix})}C_i'\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}+\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})}{S\cdot\mathbf{oc}_{mix}}\cdot C_0'\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}$$

Then simplifying yields:

(8)

$$\frac{dC'}{dt}=\frac{M\cdot\mathbf{oc}_{dep}}{S\cdot\mathbf{oc}_{mix}}C_i'\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}-\frac{M\cdot\mathbf{oc}_{dep}}{S\cdot\mathbf{oc}_{mix}}\cdot C_0'\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}-kC_0'\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}$$

and simplifying again yields

(9)

$$\frac{dC'}{dt}=(\frac{M\cdot\mathbf{oc}_{dep}}{S\cdot\mathbf{oc}_{mix}}C_i'-\frac{M\cdot\mathbf{oc}_{dep}}{S\cdot\mathbf{oc}_{mix}}\cdot C_0'-kC_0')\cdot e^{\frac{-(kS\cdot\mathbf{oc}_{mix}+M\cdot\mathbf{oc}_{dep})t}{S\cdot\mathbf{oc}_{mix}}}$$

which is the form of the original model adjusted for organic carbon concentration.